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AND STOCHASTIC EQUATIONS
— THE “PLAIN VANILLA”
GALERKIN CASE



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To be or not to be intrusive?
The solution of parametric
and stochastic equations
— the “plain vanilla” Galerkin case*

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Abstract

In parametric equations—stochastic equations are a special case—one may want to approximate the solution such that it is easy to evaluate its dependence of the parameters. Interpolation in the parameters is an obvious possibility, in this context often labeled as a collocation method. In the frequent situation where one has a “solver” for the equation for a given parameter value—this may be a software component or a program—it is evident that this can independently solve for the parameter values to be interpolated. Such *uncoupled* methods which allow the use of the original solver are classed as “non-intrusive”. By extension, all other methods which produce some kind of *coupled* system are often—in our view prematurely—classed as “intrusive”. We show for simple Galerkin formulations of the parametric problem—which generally produce coupled systems—how one may compute the approximation in a *non-intrusive* way.

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1 Introduction

Many problems depend on parameters, which may be a finite set of numerical values, or mathematically more complicated objects like for example processes or fields. We address the situation where we have an equation which depends on parameters; stochastic equations are a special case of such parametric problems where the parameters are elements from a probability space. One common way to represent this dependability on parameters is by evaluating the state (or solution) of the system under investigation for different values of the parameters. Particularly in the stochastic context this “sampling” is a common procedure. But often one wants to evaluate the solution quickly for a new set of parameters where it has not been sampled. In this situation it may be advantageous to express the parameter dependent solution with an approximation which allows for rapid evaluation of the solution or functionals thereof—so called quantities of interest (QoI)—in dependence of the parameters. Such approximations are also called *proxy* or *surrogate* models, *response functions*, or *emulators*. This last term was chosen so as to contrast with *simulator*, which is the original solver for the full equation. Such approximations are used in several fields, notably optimisation and uncertainty quantification, where in the last case the parameters are random variables and one deals with stochastic equations. All these methods may be seen as *functional approximations* — representations of the solution by an “easily computable” function of the parameters, as opposed to pure *samples*.

The most obvious methods of approximation used are based on interpolation, in this context often labelled as *collocation methods*. In this case it is usually assumed that the parameters are in some sub-domain of a manifold, usually simply just in some finite-dimensional vector space, and the interpolation is often on *sparse grids* [4, 2, 23, 49]. This process normally gives the approximation (interpolant) as a finite linear combination of some basis functions used for the interpolation, often global multi-variate polynomials [51], or piecewise polynomials [3, 48], or methods based on radial basis functions, kriging, or neural networks.

Another approach is to again choose a similar finite set of basis functions, but rather than interpolation use some other projection onto the subspace spanned by these functions. Usually this will involve minimising some norm of the difference between the true parametric solution and the approximation, and in many cases this norm will be induced by an inner product, often in the form of an integral w.r.t. some measure—in the case of stochastic equations this will be the underlying probability measure. These integrals in turn may be numerically evaluated through quadrature formulas—often again on sparse *Smolyak* or adaptive grids [42, 25, 43, 29, 24]—which need

evaluations of the integrand—part of which is the parametric solution—at a finite number of parameter values. Such methods are sometimes called *pseudo-spectral projections*, or *regression solutions*, or *discrete projections* [11, 14, 39, 10, 44, 6, 28, 5, 45].

In the frequent situation where one has a “solver” for the equation for a given parameter value, i.e. a software component or a program, it is evident that this can be used to independently—i.e. if desired in parallel—solve for all the parameter values which subsequently may be used either for the interpolation or in the quadrature for the projection. Such methods are therefore *uncoupled* for each parameter value, and obviously allow to use the original solver. Therefore, they additionally often carry the label “non-intrusive”. Without much argument all other methods—which produce a coupled system of equations—are almost always labelled as “intrusive”, meaning that one cannot use the original solver, e.g. [18, 27, 46, 19, 17]. We want to show here that this not necessarily the case.

Like most methods which are based on the solution at discrete parameter values, the non-intrusive methods mentioned above “forget” the original equation, i.e. the fact that the approximation has to satisfy the parametric equation. This is generally the state of affairs when using the proxy model in the domain of optimisation. On the other hand, methods which try to ensure that the approximation satisfies the parametric equation as well as possible are often based on a Rayleigh-Ritz or Galerkin type of “ansatz”, which leads to a *coupled* system for the unknown coefficients [26, 33, 50, 3, 34, 22, 47, 32, 12]. This is often taken as an indication that the original solver can not be used, i.e. that these methods are “intrusive”. But in many circumstances these methods may as well be used in a *non-intrusive* fashion. Although there are some publications concerning special cases of non-intrusive Galerkin-like methods [1, 13, 15], this has not been widely recognised as a general possibility. A kind of in-between possibility is the so-called *reduced basis method*, see [7, 8] for recent expositions. Here a new basis for the parametric solution is built from solves at particular parameter values, but the “interpolation” is achieved by a Galerkin projection onto the spanned subspace. This method also establishes a connection between proxy models and reduced order models, something we will not pursue further here.

Recent developments for *low-rank separated* approximations [21, 9, 30, 40, 16, 41, 20] of parametric or stochastic equations are based on the minimisation of a least squares or similar functional, and naturally lead to Galerkin-type equations. Although it is important to show that these can also be dealt with in a non-intrusive manner, here we concentrate on the “plain vanilla”, i.e. standard, Galerkin case. Non-intrusive computation of separated approx-

imations will be investigated elsewhere.

Most of the literature cited so far is concerned with the case of stochastic equations, and although these are a special case of parametric equations, the methods and techniques used there may be used in the wider context of general parametric equations, see [38] for a synopsis of these connections of such parametric problems.

The question whether a method is intrusive or not is often very important in practise. The “solver” (for a single parameter value) may contain much specialised knowledge, and may therefore represent quite a valuable investment of effort. In case the method is labelled intrusive, it may seem like the whole—often very domain specific—process and effort of producing a solver, now for the coupled Galerkin system, would have to be repeated again. Therefore, in many cases the wish to re-use existing software guides the choice of method. But as already mentioned, some very effective new methods based on low-rank approximations fall in the class of “not obviously non-intrusive” methods; hence as a first step we show here that the simple “plain vanilla” coupled Galerkin method may be computed non-intrusively, the low-rank approximation case will be treated elsewhere.

A method for a parametric problem will be here considered intrusive if one has to modify the original software to solve the parametric problem. Thus it turns out that the question of whether a method is intrusive or not hinges on what kind of interface one has to the software, and is thus a software-engineering question. Most often it is possible to not only compute the solution for a certain parameter value—the solver being usually iterative—but also the residuum or a “preconditioned residuum” given a “trial solution”. This usually means—for the preconditioned residuum—doing just one iteration with the solver instead of iterating all the way to convergence. This is the kind of interface which will be assumed here, and we shall show that this can be used without any change to solve the Galerkin equation.

The plan for the rest of the paper is as follows: In the following Section 2 we introduce the notation and assumptions for the parametric problem. In Section 3 we introduce the Galerkin approximation, describe alternative formulations, and prove the convergence and speed of a basic *block-Jacobi* algorithm for the coupled Bubnov-Galerkin system. In the Section 4 it is shown how the residual in the iteration may be computed *non-intrusively*, mainly via numerical integration. The behaviour of the modified iterates is analysed, and it is shown that they accumulate in the vicinity of the solution. A small numerical example is investigated in Section 5, it shows how the non-intrusive computation works, and it confirms the theoretical predictions.

2 Parametric Problems

To be more specific, let us consider the following situation: we are investigating some physical system which is modelled by an equation for its state $u \in \mathcal{U}$ — a Hilbert space for the sake of simplicity,

$$A(p; u) = f(p), \quad (1)$$

where A is an operator modelling the physics of the system, and $f \in \mathcal{U}^*$ is some external influence (action / excitation / loading). The model depends on some parameters $p \in \mathcal{P}$. In many cases Eq. (1) is the abstract formulation of a partial differential equation. But for the sake of simplicity we shall assume here that we are dealing with a model on a finite-dimensional space \mathcal{U} with $N := \dim \mathcal{U}$, e.g. a partial differential equation after discretisation. For simplicity we will identify \mathcal{U} and \mathcal{U}^* , and if needed we will use an orthonormal basis $\{v_n\}_{n=1}^N$, i.e. $\text{span}\{v_n\}_{n=1}^N = \mathcal{U}$ and $\langle v_n, v_m \rangle_{\mathcal{U}} = \delta_{n,m}$, the Kronecker- δ .

Assume that for all $p \in \mathcal{P}$, Eq. (1) is a well-posed problem. This means that A as a mapping $u \mapsto A(p; u)$ for a fixed p is bijective and continuously invertible, i.e. for each p and f it has a unique solution, which will be denoted by $u^*(p)$, such that for all p : $A(p; u^*(p)) = f(p)$.

Although this will not be needed here, let us remark that if the map A were also differentiable w.r.t. u , well-posedness implies that this partial derivative $D_u A$ is non-singular and also continuously invertible. Now — if the set \mathcal{P} has a differentiable structure, e.g. if it is a differentiable manifold or even a vector space — one may invoke a version of the implicit function theorem, which, given the partial derivatives $D_p A$ and $D_p f$, provides the derivative of the state u w.r.t. p as $D_p u = [D_u A]^{-1}(D_p f - D_p A)$. This — and higher derivatives — may be directly used in the approximation of $u^*(p)$, as well as for a priori bounds for some approximations. These topics will not be pursued further here.

Furthermore assume that we are also given an iterative solver — convergent for all values of p — which generates successive iterates for $k = 0, \dots$,

$$u^{(k+1)}(p) = S(p; u^{(k)}(p), R(p; u^{(k)}(p))), \quad \text{with } u^{(k)}(p) \rightarrow u^*(p), \quad (2)$$

where S is one cycle of the solver which may also depend on the iteration counter k , $u^{(0)}$ is some starting vector, and $R(p; u^{(k)}(p))$ is the residuum of Eq. (1)

$$R(u^{(k)}) := R(p; u^{(k)}(p)) := f(p) - A(p; u^{(k)}). \quad (3)$$

Obviously, when the residuum vanishes — $R(p; u^*(p)) = 0$ — the mapping S has a fixed point $u^*(p) = S(p; u^*(p), 0)$.

This mapping S is the mathematical formalisation of the software interface we will be assuming in order to derive a non-intrusive Galerkin method, i.e. we will assume that the mapping S is applied to its inputs with one invocation of the “solver”.

In the iteration in Eq. (2) we may set $u^{(k+1)} = u^{(k)} + \Delta u^{(k)}$ with

$$\Delta u^{(k)} := S(p; u^{(k)}, R(p; u^{(k)})) - u^{(k)}, \quad \text{and usually} \quad (4)$$

$$P(\Delta u^{(k)}) = R(p; u^{(k)}), \quad (5)$$

so that in Eq. (2): $S(p; u^{(k)}) = u^{(k)} + P^{-1}(R(p; u^{(k)}))$, where by slight abuse of notation we have shortened the list of arguments. Here P is some preconditioner, which may depend on p , the iteration counter k , and on the current iterate $u^{(k)}$; e.g. in *Newton's method* $P = D_u A(p; u^{(k)})$. In any case, we assume that for all arguments the map P is linear in Δu and non-singular. The iteration corresponding to a normal solve for a particular value of p then is given in Algorithm 2.1.

Algorithm 2.1 Iteration of Eq. (2)

Start with some initial guess $u^{(0)}$

$k \leftarrow 0$

while *no convergence* **do**

▷ %comment: the global iteration loop%

Compute $\Delta u^{(k)}$ according to Eq. (4) or Eq. (5)

$u^{(k+1)} \leftarrow u^{(k)} + \Delta u^{(k)}$

$k \leftarrow k + 1$

end while

We will assume additionally that the iteration converges at least linearly, i.e. one has $\|\Delta u^{(k+1)}(p)\|_{\mathcal{U}} \leq \varrho(p) \|\Delta u^{(k)}(p)\|_{\mathcal{U}}$, with $\varrho(p) < 1$. For the convergence analysis to follow later we will assume that the convergence factors or Lipschitz constants $\varrho(p)$ are uniformly bounded for all values of $p \in \mathcal{P}$ by a constant strictly less than unity, i.e. $\varrho(p) \leq \varrho^* < 1$. Another way of saying this is that for all $u, v \in \mathcal{U}$ and $p \in \mathcal{P}$ the iterator S in Eq. (2) is uniformly Lipschitz continuous with Lipschitz constant $\varrho^* < 1$, i.e. a strict contraction:

$$\|S(p; u(p), R(p; u(p))) - S(p; v(p), R(p; v(p)))\|_{\mathcal{U}} \leq \varrho^* \|u(p) - v(p)\|_{\mathcal{U}}. \quad (6)$$

One may recall from Banach's fixed point theorem that this provides us with the a posteriori error bounds

$$\|u^*(p) - u^{(k+1)}(p)\|_{\mathcal{U}} \leq \frac{\varrho^*}{1 - \varrho^*} \|\Delta u^{(k)}(p)\|_{\mathcal{U}}, \quad (7)$$

while the satisfaction of the equation may be gauged by $\|R(p; u^{(k)})\|_{\mathcal{U}}$.

3 Galerkin approximation of parametric dependence

To describe the dependence of u on the parameters p one would like to approximate $u^*(p)$ in the following fashion:

$$u^*(p) \approx u_{\mathcal{I}}(p) = \sum_{\alpha \in \mathcal{I}} u_{\alpha} \psi_{\alpha}(p), \quad (8)$$

where $u_{\alpha} \in \mathcal{U}$ are vector coefficients to be determined, and ψ_{α} are some linearly independent functions, whose linear combinations $\mathcal{Q}_{\mathcal{I}} := \text{span}\{\psi_{\alpha}\}_{\alpha \in \mathcal{I}} \subset \mathbb{R}^{\mathcal{P}}$ form the Galerkin subspace of parametric “ansatz” functions, and \mathcal{I} is some finite set of (multi-)indices of cardinality $M := |\mathcal{I}|$. Often the set \mathcal{I} has no canonical order, but for the purpose of computation later we will assume that some particular ordering has been chosen.

If we take the *ansatz* Eq. (8) and insert it into Eq. (1), the residuum Eq. (3) will usually not vanish for all p , as the finite set of functions $\{\psi_{\alpha}\}_{\alpha \in \mathcal{I}}$ can not match all possible parametric variations of $u(p)$.

3.1 The Galerkin equations for the residual

The *Galerkin* method — also called the method of weighted residuals — determines the unknown coefficients u_{α} in Eq. (8) by requiring that for all $\beta \in \mathcal{I}$

$$\mathbf{G}_{\mathcal{Q}}(\varphi_{\beta}(\cdot)R(\cdot; u_{\mathcal{I}})) = 0, \quad (9)$$

where $\{\varphi_{\beta}\}_{\beta \in \mathcal{I}}$ is a set of linearly independent functions of p . The residuum $R(p; u_{\mathcal{I}}(p))$ in the argument of the linear Galerkin projector $\mathbf{G}_{\mathcal{Q}}$ is a parametric function, and such functions may be represented by a sum $R(p; u_{\mathcal{I}}(p)) = \sum_n \phi_n(p)v_n$ with $\phi_n \in \mathbb{R}^{\mathcal{P}}$. Hence the projector may be defined by requiring that for scalar functions $\psi, \phi \in \mathcal{Q} \subseteq \mathbb{R}^{\mathcal{P}}$ and a vector $v \in \mathcal{U}$ one has

$$\mathbf{G}_{\mathcal{Q}}(\phi(\cdot)\psi(\cdot)v) = \langle \phi, \psi \rangle_{\mathcal{Q}} v, \quad (10)$$

where $\langle \cdot, \cdot \rangle_{\mathcal{Q}}$ is some duality pairing or inner product on a subspace \mathcal{Q} of the scalar functions, and from this $\mathbf{G}_{\mathcal{Q}}$ can be extended by linearity:

$$\mathbf{G}_{\mathcal{Q}}(\varphi_{\beta} R(\cdot; u_{\mathcal{I}})) = \mathbf{G}_{\mathcal{Q}}(\varphi_{\beta} \sum_n \phi_n v_n) = \sum_n \mathbf{G}_{\mathcal{Q}}(\varphi_{\beta} \phi_n v_n) = \sum_n \langle \varphi_{\beta}, \phi_n \rangle_{\mathcal{Q}} v_n.$$

It is easy to see that this definition is independent of the particular representation of the parametric function.

In case \mathcal{P} is a measure space with measure μ , then that pairing often is $\langle \phi, \psi \rangle_{\mathcal{Q}} = \int_{\mathcal{P}} \phi(p) \psi(p) \mu(dp)$, and if $\mu(\mathcal{P}) = 1$, such that \mathcal{P} may be considered as a probability space with expectation operator $\mathbb{E}(\phi) = \int_{\mathcal{P}} \phi(p) \mu(dp)$, then $\langle \phi, \psi \rangle_{\mathcal{Q}} = \mathbb{E}(\phi \psi)$. Observe that a sum like $\langle \phi, \psi \rangle_{\mathcal{Q}} = \sum_j w_j \phi(p_j) \psi(p_j)$ with positive weights w_j is a special form of such an integral. A bit more general would be to allow $\langle \phi, \psi \rangle_{\mathcal{Q}} = \iint_{\mathcal{P} \times \mathcal{P}} \kappa(p, q) \phi(p) \psi(q) \mu(dp) \mu(dq)$, where κ is a symmetric positive definite kernel. What is important for what is to follow, and what we want to assume from now on, is that the pairing is given by some integral, and we will assume the form $\int_{\mathcal{P}} \phi(p) \psi(p) \mu(dp)$ for the sake of simplicity.

The set $\{\psi_{\alpha}\}_{\alpha \in \mathcal{I}}$ determines the Galerkin subspace $\mathcal{Q}_{\mathcal{I}} := \text{span}\{\psi_{\alpha}\}_{\alpha \in \mathcal{I}} \subseteq \mathcal{Q}$, which is responsible for the approximation properties, whereas the set $\{\varphi_{\beta}\}_{\beta \in \mathcal{I}}$ determines the projection onto that subspace which is important for the stability of the procedure, as the projection is orthogonal to $\hat{\mathcal{Q}}_{\mathcal{I}} := \text{span}\{\varphi_{\beta}\}_{\beta \in \mathcal{I}}$. Often one takes $\varphi_{\beta} = \psi_{\beta}$ and hence $\hat{\mathcal{Q}}_{\mathcal{I}} = \mathcal{Q}_{\mathcal{I}}$, and this is then commonly called the *Bubnov-Galerkin* method, whereas in the general case $\hat{\mathcal{Q}}_{\mathcal{I}} \neq \mathcal{Q}_{\mathcal{I}}$ one speaks of the *Petrov-Galerkin* method.

Explicitly writing down Eq. (9), one obtains for all β

$$\mathbf{G}_{\mathcal{Q}}(\varphi_{\beta}(\cdot)(f(p) - A(p; \sum_{\alpha \in \mathcal{I}} u_{\alpha} \psi_{\alpha}(p)))) = 0. \quad (11)$$

It is important to recognise that Eq. (11) is a — usually coupled — system of equations for the unknown vectors u_{α} of size $M \times N$, as $M = \dim \mathcal{Q}_{\mathcal{I}}$ and $N = \dim \mathcal{U}$. These equations look sufficiently different from Eq. (1), so that the common wisdom is that the solution of Eq. (11) requires new software and new methods, and that the solver Eq. (2) is of no use here. As a change or re-write of the existing software seems to be necessary, the resulting methods are often labelled “intrusive”.

As a remark, observe that if one chooses $\varphi_{\beta}(p) = \delta_{\beta}(p) = \delta(p - p_{\beta})$ — the delta-“function” associated to the duality pairing $\langle \cdot, \cdot \rangle_{\mathcal{Q}}$ (i.e. $\langle \delta_{\beta}, \phi \rangle_{\mathcal{Q}} = \phi(p_{\beta})$) — where the p_{β} are distinct points in \mathcal{P} in Eq. (16), this becomes for all β :

$$0 = \mathbf{G}_{\mathcal{Q}}(\delta_{\beta} R(\cdot; u_{\mathcal{I}})) = R(p_{\beta}; u_{\mathcal{I}}(p_{\beta})) = f(p_{\beta}) - A(p_{\beta}; \sum_{\alpha \in \mathcal{I}} u_{\alpha} \psi_{\alpha}(p_{\beta})) = f(p_{\beta}) - A(p_{\beta}; u_{\beta}), \quad (12)$$

where the last of these equalities holds only in case the basis $\{\psi_{\alpha}\}$ satisfies the *Kronecker- δ* property $\psi_{\alpha}(p_{\beta}) = \delta_{\alpha, \beta}$, as then $u_{\beta} = u_{\mathcal{I}}(p_{\beta})$. In this

latter case these are M uncoupled equations each of size N , and they have for each p_β the form Eq. (1) — we have recovered the *collocation* method which independently for each p_β computes u_β , using the solver Eq. (2). Such a method then obviously is non-intrusive, as the original software may be used. Thus this is often the method of choice, as often there is considerable investment in the software which performs Eq. (2), which one would like to re-use. Unfortunately this choice is very rigid as regards the subspace $\mathcal{Q}_\mathcal{I}$ and the projection orthogonal to $\hat{\mathcal{Q}}_\mathcal{I}$.

We believe that this is a *false* alternative, and that the distinction is not between *intrusive* or *non-intrusive*, but between *coupled* or *uncoupled*. Furthermore, and more importantly, we want to show that also in the more general case of a coupled system like in Eq. (11) the original solver Eq. (2) may be put to good use. This will be achieved by making Eq. (2) the starting point, instead of Eq. (1) or Eq. (3). Such coupled iterations also arise for example from multi-physics problem, and there these coupled iterations can also be solved by what is called a *partitioned* approach, see e.g. [35], which is the equivalent of non-intrusive here. Quite a number of different variants of global partitioned iterations are possible [35], we only look at some of the simplest variants, as the point is here only to dispel the myth about intrusiveness.

3.2 The fixed-point Galerkin equations

Whatever the starting point, we would still like to achieve the same result. So before continuing, let us show

Proposition 1. *Projecting the fixed point equation attached to the iteration Eq. (2), namely $u_\mathcal{I} = u_\mathcal{I} + P^{-1}(R(u_\mathcal{I}))$, is equivalent to projecting the preconditioned residual $P^{-1}(R(u_\mathcal{I}))$, that means for all $\beta \in \mathcal{I}$*

$$\mathbf{G}_\mathcal{Q}(\varphi_\beta(\cdot) P^{-1}(\cdot)(R(\cdot; u_\mathcal{I}(\cdot)))) = 0. \quad (13)$$

Moreover, if the preconditioner P in Eq. (5) does not depend on p nor u , then it is equivalent to projecting the residual $R(u_\mathcal{I})$ from Eq. (9), that means for all $\beta \in \mathcal{I}$

$$\mathbf{G}_\mathcal{Q}(\varphi_\beta(\cdot) R(\cdot; u_\mathcal{I}(\cdot))) = 0. \quad (14)$$

Proof. The Eq. (13) follows simply from linearity of $\mathbf{G}_\mathcal{Q}$. Furthermore, in case P does not depend on p nor u , for Eq. (14) we have from Eq. (13) for any $\beta \in \mathcal{I}$

$$\begin{aligned} 0 &= \mathbf{G}_\mathcal{Q}(\varphi_\beta(\cdot) P^{-1}(R(\cdot; u_\mathcal{I}(\cdot)))) = P^{-1} \mathbf{G}_\mathcal{Q}(\varphi_\beta R(u_\mathcal{I})) \\ &\Leftrightarrow 0 = \mathbf{G}_\mathcal{Q}(\varphi_\beta R(u_\mathcal{I})), \end{aligned} \quad (15)$$

on noting that for any linear map L one has $\mathbf{G}_{\mathcal{Q}}(\varphi(\cdot)L(\phi(\cdot)v)) = \langle \varphi, \phi \rangle_{\mathcal{Q}} Lv = L \mathbf{G}_{\mathcal{Q}}(\varphi(\cdot)\phi(\cdot)v)$, and by observing that P^{-1} is non-singular. \square

This means that instead of the residual Eq. (3) we may just as well project the iteration Eq. (5): with the abbreviation $R^{(k)}(\cdot) := R(\cdot; u^{(k)}(\cdot))$ we have for all $\beta \in \mathcal{I}$

$$\mathbf{G}_{\mathcal{Q}}(\varphi_{\beta}(\cdot)u^{(k+1)}) = \mathbf{G}_{\mathcal{Q}}(\varphi_{\beta}(u^{(k)} + \Delta u^{(k)})) = \mathbf{G}_{\mathcal{Q}}(\varphi_{\beta}(u^{(k)} + P^{-1}R^{(k)})). \quad (16)$$

Expanding $u^{(k)}(p) = \sum_{\alpha} u_{\alpha}^{(k)} \psi_{\alpha}(p)$ in Eq. (16), that becomes a coupled iteration equation for the u_{α} :

$$\forall \beta : \mathbf{G}_{\mathcal{Q}}(\varphi_{\beta}(\cdot) \sum_{\alpha} u_{\alpha}^{(k+1)} \psi_{\alpha}(\cdot)) = \mathbf{G}_{\mathcal{Q}}(\varphi_{\beta}(\cdot) (\sum_{\alpha} u_{\alpha}^{(k)} \psi_{\alpha}(\cdot) + P^{-1}R^{(k)}(\cdot))), \quad (17)$$

which may now be written as

$$\forall \beta : \sum_{\alpha} \mathbf{M}_{\beta, \alpha} u_{\alpha}^{(k+1)} = \sum_{\alpha} \mathbf{M}_{\beta, \alpha} u_{\alpha}^{(k)} + \mathbf{G}_{\mathcal{Q}}(\varphi_{\beta} P^{-1}R^{(k)}), \quad (18)$$

where $\mathbf{M}_{\beta, \alpha} := \langle \varphi_{\beta}, \psi_{\alpha} \rangle_{\mathcal{Q}}$. If the coefficients $u_{\alpha}^{(k)} \in \mathcal{U}$ are arranged column-wise in a $N \times M$ matrix $\mathbf{u}^{(k)} = [\dots, u_{\alpha}^{(k)}, \dots] \in \mathcal{U}^{\mathcal{I}}$ and similarly $\mathbf{G}_{\mathcal{Q}}(P^{-1}R^{(k)}) = [\dots, \mathbf{G}_{\mathcal{Q}}(\varphi_{\alpha} P^{-1}R^{(k)}), \dots]$, and the $\mathbf{M}_{\beta, \alpha}$ are viewed as entries of a $M \times M$ matrix $\mathbf{M} \in \mathbb{R}^{\mathcal{I} \times \mathcal{I}}$, Eq. (18) may be compactly written as

$$\mathbf{u}^{(k+1)} \mathbf{M}^T = \mathbf{u}^{(k)} \mathbf{M}^T + \mathbf{G}_{\mathcal{Q}}(P^{-1}R^{(k)}), \quad \text{or as} \quad (19)$$

$$\mathbf{u}^{(k+1)} = \mathbf{u}^{(k)} + \Delta_{\mathcal{Q}}(\mathbf{u}^{(k)}) =: \mathbf{S}_{\mathcal{Q}}(\mathbf{u}^{(k)}), \quad (20)$$

where we have defined two new functions $\Delta_{\mathcal{Q}}(\mathbf{u}^{(k)}) := [\mathbf{G}_{\mathcal{Q}}(P^{-1}R^{(k)})] \mathbf{M}^{-T}$, and $\mathbf{S}_{\mathcal{Q}}(\mathbf{u}^{(k)}) = \mathbf{u}^{(k)} + \Delta_{\mathcal{Q}}(\mathbf{u}^{(k)})$, which will be needed later for the convergence analysis in Subsection 3.3.

It is apparent that the computation will be much simplified if the ansatz-functions $\{\psi_{\alpha}\}_{\alpha \in \mathcal{I}}$ and the test-functions for the projection $\{\varphi_{\beta}\}_{\beta \in \mathcal{I}}$ are chosen bi-orthogonal, i.e. if one has for all $\alpha, \beta \in \mathcal{I}$ that $\mathbf{M}_{\beta, \alpha} = \delta_{\beta, \alpha}$, i.e. $\mathbf{M} = \mathbf{I}$, which shall be assumed from now on. Hence now

$$\Delta_{\mathcal{Q}}(\mathbf{u}^{(k)}) = \mathbf{G}_{\mathcal{Q}}(P^{-1}R^{(k)}) = [\dots, \mathbf{G}_{\mathcal{Q}}(\varphi_{\alpha} P^{-1}R^{(k)}), \dots]. \quad (21)$$

Eq. (20) is already a possible way of performing the iteration. The practical, non-intrusive, computation of the terms in Eq. (20) still has to be

considered, but we may formulate the corresponding Algorithm 3.1 and investigate its convergence beforehand. The reader who is only interested in the computational description of the non-intrusive algorithm may jump directly to Section 4.

Algorithm 3.1 Block Jacobi iteration of Eq. (20)

```

Start with some initial guess  $\mathbf{u}^{(0)}$ 
 $k \leftarrow 0$ 
while no convergence do
     $\triangleright$  %comment: the global iteration loop%
    Compute  $\Delta_{\mathcal{Q}}(\mathbf{u}^{(k)})$  according to Eq. (21)
     $\mathbf{u}^{(k+1)} \leftarrow \mathbf{u}^{(k)} + \Delta_{\mathcal{Q}}(\mathbf{u}^{(k)})$  [ $= \mathbf{S}_{\mathcal{Q}}(\mathbf{u}^{(k)})$ ]
     $k \leftarrow k + 1$ 
end while

```

Although the underlying iteration Eq. (2) in Algorithm 2.1 may be of any kind — e.g. Newton’s method — when one views Eq. (20) with regard to the block structure imposed by the $\mathbf{u} = [\dots, u_{\beta}, \dots]$, Algorithm 3.1 is a — maybe nonlinear — *block Jacobi* iteration.

3.3 Convergence of coupled iterations

Here we want to show that the map $\mathbf{S}_{\mathcal{Q}}$ in Eq. (20) satisfies a Lipschitz condition with the same constant as in Eq. (6). This will need some more theoretical considerations. For the sake of simplicity we will assume that $\langle \cdot, \cdot \rangle_{\mathcal{Q}}$ is actually an inner product on the Hilbert space $\mathcal{Q} \subseteq \mathbb{R}^{\mathcal{P}}$, such that $\mathcal{Q}_{\mathcal{I}} \subseteq \mathcal{Q}$. The contraction condition for $\mathbf{S}_{\mathcal{Q}}$ with contraction factor (Lipschitz constant) less or equal to ϱ^* will only hold if the Galerkin projection is *orthogonal*, i.e. we have to take $\varphi_{\alpha} = \psi_{\alpha}$, which means $\hat{\mathcal{Q}}_{\mathcal{I}} = \mathcal{Q}_{\mathcal{I}}$. Our previous assumption that $\mathbf{M} = \mathbf{I}$ — which is now the Gram matrix of the basis $\{\psi_{\alpha}\}_{\alpha \in \mathcal{I}}$ — now means that this basis is actually *orthonormal*.

Parametric elements like $\mathcal{P} \ni p \mapsto u(p) \in \mathcal{U}$ are formally in the Hilbert tensor product space of sums like $\sum_n \phi_n(p) v_n =: \sum \phi_n \otimes v_n \in \mathcal{Q} \otimes \mathcal{U}$, with the inner product of two elementary tensors $\phi_j \otimes w_j \in \mathcal{Q} \otimes \mathcal{U}$, ($j = 1, 2$), defined by $\langle \phi_1 \otimes w_1, \phi_2 \otimes w_2 \rangle_{\mathcal{Q} \otimes \mathcal{U}} := \langle \phi_1, \phi_2 \rangle_{\mathcal{Q}} \langle w_1, w_2 \rangle_{\mathcal{U}}$, and then extended by bilinearity. In the space \mathcal{Q} , the subspace $\mathcal{Q}_{\mathcal{I}}$, which is finite-dimensional and hence closed, leads to the orthogonal direct sum decomposition $\mathcal{Q} = \mathcal{Q}_{\mathcal{I}} \oplus \mathcal{Q}_{\mathcal{I}}^{\perp}$, and hence to the orthogonal direct sum decomposition $\mathcal{Q} \otimes \mathcal{U} = (\mathcal{Q}_{\mathcal{I}} \otimes \mathcal{U}) \oplus (\mathcal{Q}_{\mathcal{I}}^{\perp} \otimes \mathcal{U})$.

The mapping $J : \mathcal{U}^{\mathcal{I}} \ni \mathbf{u} = [\dots, u_{\alpha}, \dots] \mapsto \sum_{\alpha} \psi_{\alpha}(\cdot) u_{\alpha} \in \mathcal{Q}_{\mathcal{I}} \otimes \mathcal{U} \subseteq \mathcal{Q} \otimes \mathcal{U}$

is by design bijective onto $\mathcal{Q}_{\mathcal{I}} \otimes \mathcal{U}$ and may thus be used to induce a norm and inner product on $\mathcal{U}^{\mathcal{I}}$ via $\|\mathbf{u}\|_{\mathcal{U}^{\mathcal{I}}}^2 := \|J\mathbf{u}\|_{\mathcal{Q} \otimes \mathcal{U}}^2 = \|\sum_{\alpha} \psi_{\alpha}(\cdot) u_{\alpha}\|_{\mathcal{Q} \otimes \mathcal{U}}^2 = \sum_{\alpha} \|u_{\alpha}\|_{\mathcal{U}}^2$, making it a unitary map, hence $\|J\| = 1$. When viewed as a mapping into the larger space $\mathcal{Q} \otimes \mathcal{U}$, were it is extended by slight abuse of notation by the inclusion, it remains an isometry.

Lemma 2. *The maps $\mathbf{G}_{\mathcal{Q}} : \mathcal{Q} \otimes \mathcal{U} \rightarrow \mathcal{U}^{\mathcal{I}}$ and J are adjoints of each other, $\mathbf{G}_{\mathcal{Q}}^* = J$, and $\mathbf{G}_{\mathcal{Q}}$ is non-expansive, $\|\mathbf{G}_{\mathcal{Q}}\| = \|\mathbf{G}_{\mathcal{Q}}^*\| = 1$.*

Proof. For all $\mathbf{v} \in \mathcal{U}^{\mathcal{I}}$ and $\phi \otimes w \in \mathcal{Q} \otimes \mathcal{U}$:

$$\begin{aligned} \langle \mathbf{G}_{\mathcal{Q}}(\phi \otimes w), \mathbf{v} \rangle_{\mathcal{U}^{\mathcal{I}}} &= \langle [\dots, \langle \psi_{\alpha}, \phi \rangle_{\mathcal{Q}} w, \dots], [\dots, v^{\alpha}, \dots] \rangle_{\mathcal{U}^{\mathcal{I}}} = \\ \sum_{\alpha} \langle \psi_{\alpha}, \phi \rangle_{\mathcal{Q}} \langle w, v^{\alpha} \rangle_{\mathcal{U}} &= \langle \phi \otimes w, \sum_{\alpha} \psi_{\alpha} \otimes v^{\alpha} \rangle_{\mathcal{Q} \otimes \mathcal{U}} = \langle \phi \otimes w, J\mathbf{v} \rangle_{\mathcal{Q} \otimes \mathcal{U}}, \end{aligned} \quad (22)$$

and hence $\mathbf{G}_{\mathcal{Q}}^* = J$. But J is an isometry, so that one has $\|\mathbf{G}_{\mathcal{Q}}^*\| = \|J\| = 1$. As $\|\mathbf{G}_{\mathcal{Q}}\| = \|\mathbf{G}_{\mathcal{Q}}^*\|$, we are finished. \square

With the observation that

$$\begin{aligned} \mathbf{G}_{\mathcal{Q}}(S(\cdot; u^{(k)}(\cdot), R^{(k)}(\cdot))) &= \mathbf{G}_{\mathcal{Q}}(u^{(k)}(\cdot) + P^{-1}R^{(k)}(\cdot)) = \\ \mathbf{u}^{(k)} + \mathbf{G}_{\mathcal{Q}}(P^{-1}R^{(k)}) &= \mathbf{u}^{(k)} + \mathbf{\Delta}_{\mathcal{Q}}(\mathbf{u}^{(k)}) = \mathbf{S}_{\mathcal{Q}}(\mathbf{u}^{(k)}), \end{aligned} \quad (23)$$

the map $\mathbf{S}_{\mathcal{Q}} : \mathcal{U}^{\mathcal{I}} \rightarrow \mathcal{U}^{\mathcal{I}}$ in Eq. (20) may be factored in the following way:

$$\mathbf{S}_{\mathcal{Q}} : \mathcal{U}^{\mathcal{I}} \xrightarrow{J} \mathcal{Q} \otimes \mathcal{U} \xrightarrow{\tilde{S}} \mathcal{Q} \otimes \mathcal{U} \xrightarrow{\mathbf{G}_{\mathcal{Q}}^*} \mathcal{U}^{\mathcal{I}}, \quad (24)$$

$$\mathbf{S}_{\mathcal{Q}} = \mathbf{G}_{\mathcal{Q}} \circ \tilde{S} \circ J = \mathbf{G}_{\mathcal{Q}} \circ \tilde{S} \circ \mathbf{G}_{\mathcal{Q}}^*, \quad (25)$$

where \tilde{S} is defined via the solver map S in Eq. (2) by

$$\tilde{S} : \mathcal{Q} \otimes \mathcal{U} \ni u(\cdot) \mapsto S(\cdot; u(\cdot), R(\cdot, u(\cdot))) \in \mathcal{Q} \otimes \mathcal{U}. \quad (26)$$

For this mapping we have the following result:

Proposition 3. *In Eq. (26), the map denoted \tilde{S} has the same Lipschitz constant ϱ^* as the map S in Eq. (2), cf. Eq. (6); i.e. \tilde{S} is a contraction with contraction factor $\varrho^* < 1$.*

Proof. We now use the assumption that the inner product on \mathcal{Q} is given by an integral, $\langle \varphi, \phi \rangle_{\mathcal{Q}} = \int_{\mathcal{P}} \varphi(p) \phi(p) \mu(\mathrm{d}p)$. In that case $\mathcal{Q} = L_2(\mathcal{P}, \mu; \mathbb{R})$, and

the Hilbert tensor product $\mathcal{Q} \otimes \mathcal{U}$ is isometrically isomorphic to $L_2(\mathcal{P}, \mu; \mathcal{U})$. Hence with Eq. (6) for all $u(\cdot), v(\cdot) \in L_2(\mathcal{P}, \mu; \mathcal{U})$

$$\begin{aligned} \|\tilde{S}(u(\cdot)) - \tilde{S}(v(\cdot))\|_{L_2(\mathcal{P}, \mu; \mathcal{U})}^2 &= \\ &= \int_{\mathcal{P}} \|S(p; u(p), R(p; u(p))) - S(p; v(p), R(p; v(p)))\|_{\mathcal{U}}^2 \mu(dp) \\ &\leq (\varrho^*)^2 \int_{\mathcal{P}} \|u(p) - v(p)\|_{\mathcal{U}}^2 \mu(dp) = (\varrho^*)^2 \|u(\cdot) - v(\cdot)\|_{L_2(\mathcal{P}, \mu; \mathcal{U})}^2, \end{aligned}$$

and the proof is concluded by taking square roots. \square

This immediately leads to

Corollary 4. *The map $\mathbf{S}_{\mathcal{Q}}$ from Eq. (20) is a contraction with contraction factor $\varrho^* < 1$ (see Eq. (6)):*

$$\forall \mathbf{u}, \mathbf{v} \in \mathcal{U}^{\mathcal{I}} : \quad \|\mathbf{S}_{\mathcal{Q}}(\mathbf{u}) - \mathbf{S}_{\mathcal{Q}}(\mathbf{v})\|_{\mathcal{U}^{\mathcal{I}}} \leq \varrho^* \|\mathbf{u} - \mathbf{v}\|_{\mathcal{U}^{\mathcal{I}}}, \quad (27)$$

and hence the Galerkin equations have a unique solution $\mathbf{u}^* \in \mathcal{U}^{\mathcal{I}}$.

Proof. This follows from the decomposition Eq. (25), Lemma 2, and Proposition 3, as $\|\mathbf{S}_{\mathcal{Q}}\| = \|\mathbf{G}_{\mathcal{Q}} \circ \tilde{S} \circ \mathbf{G}_{\mathcal{Q}}^*\| \leq \|\mathbf{G}_{\mathcal{Q}}\| \|\tilde{S}\| \|\mathbf{G}_{\mathcal{Q}}^*\| \leq \varrho^*$, and Banach's contraction mapping theorem. \square

Now we may state the main result about the convergence of the simple block-Jacobi Algorithm 3.1 for the coupled Galerkin system:

Theorem 5. *As the map $\mathbf{S}_{\mathcal{Q}}$ from Eq. (20) has Lipschitz constant $\varrho^* < 1$, and is thus a contraction with the same factor as the solver S in Eq. (2), the Algorithm 3.1 converges to the unique solution $\mathbf{u}^* \in \mathcal{U}^{\mathcal{I}}$ with the same linear speed of convergence as Algorithm 2.1. Additionally, we have the a posteriori error estimate (see Eq. (7))*

$$\|\mathbf{u}^* - \mathbf{u}^{(k+1)}\|_{\mathcal{U}^{\mathcal{I}}} \leq \frac{\varrho^*}{1 - \varrho^*} \|\Delta_{\mathcal{Q}}(\mathbf{u}^{(k)})\|_{\mathcal{U}^{\mathcal{I}}}. \quad (28)$$

The satisfaction of the parametric equation may be gauged by $\|R^{(k)}\|_{\mathcal{Q} \otimes \mathcal{U}} = \|R(\cdot; u^{(k)})\|_{\mathcal{Q} \otimes \mathcal{U}}$.

Proof. Everything simply follows from Corollary 4, Banach's contraction mapping theorem, and the fact that $R^{(k)}(\cdot)$ is the residuum at iteration k before any preconditioning or projection. \square

Observe that this only holds for the linear convergence speed; in case Algorithm 2.1 has super-linear convergence, this can not be necessarily matched by Algorithm 3.1, for this more sophisticated algorithms for the coupled equations are necessary, see e.g. [35].

4 Non-intrusive residual

Here we want to look in more detail at the actual computation of the right hand side of Eq. (20), in the form Eq. (21). One may observe that the term $\mathbf{G}_{\mathcal{Q}}(\varphi_{\alpha} P^{-1} R^{(k)})$ in Eq. (21) is the Galerkin projection of the preconditioned residual for that iteration. Let us recall that the Galerkin projector was defined by Eq. (10) as $\mathbf{G}_{\mathcal{Q}}(\varphi(\cdot) v \phi(\cdot)) = \langle \varphi, \phi \rangle_{\mathcal{Q}} v$.

4.1 Analytic computation

In some cases [38, 37], notably when the preconditioner P does not depend on p nor u , or when the operator A is linear or polynomial in u , and linear in the parameters p , it may be possible to actually represent $P^{-1} R^{(k)}$, not just in principle, but actually *non-intrusively* through the use of the solver S in Eq. (2) as

$$P^{-1} R^{(k)}(p) = \sum_n \rho_n(p) v_n = \sum_{n,\beta} \rho_{n,\beta} \psi_{\beta}(p) v_n, \quad (29)$$

where $\rho_{n,\beta} = \langle \psi_{\beta}, \rho_n \rangle_{\mathcal{Q}}$, — remembering that we chose $\varphi_{\alpha} = \psi_{\alpha}$ orthonormal. The Galerkin projection of this then gives

$$\begin{aligned} \mathbf{G}_{\mathcal{Q}}(\psi_{\alpha} P^{-1} R^{(k)}) &= \mathbf{G}_{\mathcal{Q}}(\psi_{\alpha} \sum_{n,\beta} \rho_{n,\beta} \psi_{\beta} v_n) = \\ &= \sum_{n,\beta} \rho_{n,\beta} \mathbf{G}_{\mathcal{Q}}(\psi_{\alpha} \psi_{\beta} v_n) = \sum_{n,\beta} \rho_{n,\beta} \langle \psi_{\alpha}, \psi_{\beta} \rangle_{\mathcal{Q}} v_n = \sum_n \rho_{n,\alpha} v_n, \end{aligned} \quad (30)$$

using the linearity of $\mathbf{G}_{\mathcal{Q}}$ and the orthonormality of the basis $\{\psi_{\alpha}\}_{\alpha \in \mathcal{I}}$. This means that for the right hand side of Eq. (20) in the form Eq. (21), given the representation Eq. (29), each term may be computed through simple linear algebra operations Eq. (30). This expression may be directly used in the *block-Jacobi* Algorithm 3.1 for $\Delta_{\mathcal{Q}}(\mathbf{u}^{(k)})$ in the form Eq. (21), and the description of the algorithm is complete. Let us remark finally that if the solver actually returns $S(p; u^{(k)}(p), R^{(k)}(p))$ instead of the increment $P^{-1} R^{(k)}(p)$, Algorithm 3.1 is easily adapted by computing completely analogously $\mathbf{S}_{\mathcal{Q}}(\mathbf{u}^{(k)})$.

4.2 Numerical integration

The following idea to obtain a non-intrusive computation of the right hand side of Eq. (20) in the form Eq. (21), is more general, but involves a further approximation, namely numerical integration.

Remembering that it was assumed that the duality pairing on the scalar functions is given by an integral with measure μ ,

$$\langle \varphi, \phi \rangle_{\mathcal{Q}} = \int_{\mathcal{P}} \varphi(p) \phi(p) \mu(dp), \quad (31)$$

we now assume that this integral has some approximate numerical quadrature formula

$$\int_{\mathcal{P}} \phi(p) \mu(dp) \approx \sum_{z=1}^Z w_z \phi(p_z), \quad (32)$$

where the integrand is evaluated at the quadrature points p_z and the w_z are appropriate weights.

With this approximation the term $\mathbf{G}_{\mathcal{Q}}(\psi_{\beta} P^{-1} R^{(k)})$ in Eq. (18) becomes practically computable without any further assumptions on the operator A , giving

$$\mathbf{G}_{\mathcal{Q}}(\psi_{\beta} P^{-1} R^{(k)}) \approx \Delta_{Z,\beta} u^{(k)} := \sum_z w_z \psi_{\beta}(p_z) \Delta u_z^{(k)}, \quad \text{where} \quad (33)$$

$$\Delta u_z^{(k)} := P^{-1}(p_z) R(p_z; u^{(k)}(p_z)) = P^{-1}(p_z) \left(f(p_z) - A(p_z; u^{(k)}(p_z)) \right), \quad (34)$$

$$\text{or} \quad = S(p_z; u^{(k)}(p_z), R(p_z; u^{(k)}(p_z))) - u^{(k)}(p_z) \quad (35)$$

is the preconditioned residuum evaluated at p_z , and $u^{(k)}(p_z) = \sum_{\alpha} u_{\alpha}^{(k)} \psi_{\alpha}(p_z)$. This is indeed the only interface needed to the original equation, something which can be easily evaluated *non-intrusively* as the iteration increment $\Delta u_z^{(k)}$ in Eq. (34) in case the current state is given as $u^{(k)}(p_z)$ for the parameter value p_z . An alternative form is given in Eq. (35), which is one iteration of the solver, starting at $u^{(k)}(p_z)$ for the parameter p_z . This variant is for the case when the solver actually returns $S(p; u^{(k)}(p), R^{(k)}(p))$ instead of the increment $P^{-1} R^{(k)}(p)$.

4.3 Non-intrusive iteration

The term in Eq. (20) in the form of Eq. (21) has to be computed *non-intrusively*. Following Subsection 4.2 about numerical integration of the terms — if applicable, the analytic counterpart from Subsection 4.1 can be easily substituted — we formulate the approximation of

$$\begin{aligned} \Delta_{\mathcal{Q}}(\mathbf{u}^{(k)}) &= [\dots, \mathbf{G}_{\mathcal{Q}}(\varphi_{\alpha} P^{-1} R^{(k)}), \dots] \\ &\approx \Delta_Z(\mathbf{u}^{(k)}) = [\dots, \Delta_{Z,\alpha} u^{(k)}, \dots] \end{aligned} \quad (36)$$

Algorithm 4.1 Non-intrusive computation of Eq. (21) in the form of Eq. (36)

```

for  $\alpha \in \mathcal{I}$  do
     $\Delta_{Z,\alpha} u^{(k)} \leftarrow 0$ 
end for
    ▷ %comment: the loop over integration points%
for  $z \leftarrow 1, \dots, Z$  do
    Compute  $\Delta u_z^{(k)}$  from Eq. (34)
     $r_z \leftarrow w_z \Delta u_z^{(k)}$ 
    for  $\alpha \in \mathcal{I}$  do
         $\Delta_{Z,\alpha} u^{(k)} \leftarrow \Delta_{Z,\alpha} u^{(k)} + \psi_\alpha(p_z) r_z$ 
    end for
end for

```

in Algorithm 3.1 from Eq. (21) in Algorithm 4.1, using Eq. (33) and Eq. (34):

The result of this algorithm is $\Delta_Z(\mathbf{u}^{(k)})$, the approximation of $\Delta_Q(\mathbf{u}^{(k)})$ by numerical integration. With Algorithm 4.1 it is now possible to formulate a non-intrusive version of Algorithm 3.1, the block-Jacobi iteration, in Algorithm 4.2.

Algorithm 4.2 Non-Intrusive block Jacobi iteration of Eq. (20)

```

Start with some initial guess  $\tilde{\mathbf{u}}^{(0)} = [\dots, \tilde{u}_\alpha^{(0)}, \dots]$ 
 $k \leftarrow 0$ 
while no convergence do
    ▷ %comment: the global iteration loop%
    Compute  $\Delta_Z(\tilde{\mathbf{u}}^{(k)}) = [\dots, \Delta_{Z,\alpha} \tilde{u}^{(k)}, \dots]$  according to Algorithm 4.1
     $\tilde{\mathbf{u}}^{(k+1)} \leftarrow \tilde{\mathbf{u}}^{(k)} + \Delta_Z(\tilde{\mathbf{u}}^{(k)})$ 
     $k \leftarrow k + 1$ 
end while

```

The sequence generated by Algorithm 4.2 has been labelled with a tilde $\{\tilde{\mathbf{u}}^{(k)}\}_k$ to distinguish it from the exact sequence $\{\mathbf{u}^{(k)}\}_k$ generated by Algorithm 3.1. The question arises as to how well the original sequence $\{\mathbf{u}^{(k)}\}_k$ is approximated by the one produced non-intrusively by numerical integration $\{\tilde{\mathbf{u}}^{(k)}\}_k$, and what its convergence behaviour is. To that effect we partially cite and conclude from Theorem 4.1 in [36]:

Theorem 6. *Assume that the numerical integration in Algorithm 4.1 is performed such that $\|\mathbf{G}_Q(\psi_\alpha P^{-1} R(\cdot; \tilde{u}^{(k)})) - \Delta_{Z,\alpha} \tilde{u}^{(k)}\|_U \leq \varepsilon/\sqrt{M}$, then the*

error in Eq. (36) is estimated by

$$\|\Delta_{\mathcal{Q}}(\tilde{\mathbf{u}}^{(k)}) - \Delta_Z(\tilde{\mathbf{u}}^{(k)})\|_{\mathcal{U}^{\mathcal{I}}} \leq \varepsilon, \quad (37)$$

and we have the following *a posteriori* error estimate for the iterates

$$\|\mathbf{u}^* - \tilde{\mathbf{u}}^{(k+1)}\|_{\mathcal{U}^{\mathcal{I}}} \leq \frac{\varrho^*}{1 - \varrho^*} \|\Delta_Z(\tilde{\mathbf{u}}^{(k)})\|_{\mathcal{U}^{\mathcal{I}}} + \frac{\varepsilon}{1 - \varrho^*}. \quad (38)$$

In addition, we have that

$$\limsup_{k \rightarrow \infty} \|\mathbf{u}^* - \tilde{\mathbf{u}}^{(k)}\|_{\mathcal{U}^{\mathcal{I}}} \leq \frac{\varepsilon}{1 - \varrho^*}. \quad (39)$$

The satisfaction of the parametric equation may be gauged by $\|R(\cdot; \tilde{\mathbf{u}}^{(k)})\|_{\mathcal{Q} \otimes \mathcal{U}}$.

Proof. The Eq. (37) is a simple consequence of the assumption by squaring and summing $M = |\mathcal{I}|$ terms of size less than ε/\sqrt{M} , and then taking the square root. Everything else are then statements of Theorem 4.1 in [36]. \square

The Eq. (38) shows that the modified sequence $\{\tilde{\mathbf{u}}^{(k)}\}_k$ will not necessarily converge to \mathbf{u}^* , even if $\Delta_Z(\tilde{\mathbf{u}}^{(k)}) \rightarrow 0$ as $k \rightarrow \infty$, but Eq. (39) shows that it clusters around \mathbf{u}^* in a small neighbourhood.

4.4 Computational effort and possible improvements

To assess the effort involved in a computational procedure and hence its efficiency is always difficult, not least because it is not always clear on how to measure computational effort. Here we take the view that the effort is only counted in solver calls, i.e. invocations of $S(p; u, R(p; u))$ Eq. (2) or equivalently of $P^{-1}R(p; u)$ Eq. (5). This means that the additional linear algebra and computation of $\psi_{\alpha}(p_z)$ involved in the Algorithms 4.1 and 4.2 is considered insignificant in comparison to an invocation of the solver S .

The main contender for the Galerkin procedure outlined so far is to be seen in what is called in the introduction a pseudo-spectral or discrete projection, or a regression. This can be described very quickly. With $\{\psi_{\alpha}\}_{\alpha \in \mathcal{I}}$ orthonormal, the coefficients in the projection $u_{\mathcal{I}} = \sum_{\alpha \in \mathcal{I}} u^{\alpha} \psi_{\alpha}$ can be simply computed by inner products:

$$u^{\alpha} = \langle \psi_{\alpha}, u^* \rangle_{\mathcal{Q}} = \int_{\mathcal{P}} \psi_{\alpha}(p) u^*(p) \mu(\mathrm{d}p) \approx \sum_{z=1}^Z w_z \psi(p_z) u^*(p_z). \quad (40)$$

One may remind oneself that this — being the orthogonal projection onto the subspace $\mathcal{Q}_{\mathcal{I}} \subseteq \mathcal{Q}$ — has the smallest error to $u^*(p)$ in the norm $\|\cdot\|_{\mathcal{Q}}$, but

it does not at all take into account the parametric equation. The Galerkin projection on the other hand will produce an approximation which is optimal in minimising the residuum. The approximation in Algorithm 4.3 to Eq. (40) is computed very similarly to Algorithm 4.1.

Algorithm 4.3 Discrete projection according to Eq. (40)

```

for  $\alpha \in \mathcal{I}$  do
     $u^\alpha \leftarrow 0$ 
end for
▷ %comment: the loop over integration points%
for  $z \leftarrow 1, \dots, Z$  do
    Compute  $u(p_z)$  according to Algorithm 2.1.
     $r_z \leftarrow w_z u(p_z)$ 
    for  $\alpha \in \mathcal{I}$  do
         $u^\alpha \leftarrow u^\alpha + \psi_\alpha(p_z) r_z$ 
    end for
end for

```

The iterations from Eq. (2) in Algorithm 2.1 with one solver call per iteration in Algorithm 4.3 are assumed to be contractions with contraction factor at most ϱ^* . Say that an iteration with contraction factor of ϱ^* needs L iterations to converge to the desired accuracy. The discrete projection needs L solver calls on Z integration points each, i.e. $L \times Z$ solver calls.

The block Jacobi variant of the coupled Galerkin system in Algorithm 4.2 needs *one* solver call on Z integration points. But as it converges also with contraction factor ϱ^* — see Corollary 4, it also needs L iterations, i.e. in total also $L \times Z$ solver calls.

We see that in this measure of effort — solver calls — the discrete projection and the block Jacobi iteration of the Galerkin system need the same effort for comparable accuracy; something that is borne out also in the numerical example in Section 5. In case the iteration in Eq. (2) is quadratically convergent, e.g. it is Newton’s method, then this can not be matched by the block Jacobi method; it will usually only have linear convergence. When looking at the other computations apart from the count of solver calls, in both algorithms integrals have to be approximated by quadrature formulas. In the discrete projection this happens only once, whereas in the block Jacobi this is done in every global iteration.

Block Jacobi is probably the simplest method for coupled systems, however it can be considerably accelerated [31, 35], this ranges from the simple *Aitken* acceleration over block *Gauss-Seidel* to *Quasi-Newton* methods. In

case the iterations from Eq. (2) converge only linearly, these extensions can then produce an advantage for the Galerkin solution and may need considerably fewer than L iterations, as “convergence information” is shared for different values of p or α , something which will not happen in the decoupled discrete projection. Even *Newton’s* method [31] can be emulated on the global Galerkin system, where the action of the inverse of the derivative on a vector is approximated by finite differences and non-intrusive solver calls. This last procedure is even able to maintain quadratic convergence in case the iterations from Eq. (2) are quadratically convergent themselves. These issues will be taken up and published elsewhere.

Another area where considerable saving of work is possible in the Galerkin procedure are sparse or low-rank approximations. They come about when viewing the solution — and also other parametric elements — as *tensors*, which may be used computationally in *low-rank* representations / approximations, see for example [36]. Again this is beyond the scope of the present paper, and will be published elsewhere. Using such low-rank representations in the originally uncoupled discrete projection produces a coupled system, which then differs not substantially from the Galerkin system. Other ways of building a low-rank representation were already discussed in the introduction, and will be the subject of a future paper.

5 Numerical example

Here we want to show the procedures discussed on a tiny example which nonetheless is representative of parametric problems. It is so simple that it may be programmed with a few lines of code. This computational example derives from a little electrical resistor network with a global non-linearity. The particular resistor network we use is shown in Fig. 1.

Kirchhoff’s and Ohm’s laws lead to the following linear relation between voltages \mathbf{u} and currents \mathbf{j} fed into the nodes, where the numbering of the nodes corresponds to the equations — node 6 is grounded ($u_6 = 0$) and so needs no equation, hence $\mathbf{u} \in \mathcal{U} = \mathbb{R}^5$, $\mathbf{K} \in \mathbb{R}^{5 \times 5}$:

$$\mathbf{K}\mathbf{u} = \mathbf{j}, \quad (41)$$

with

$$\mathbf{K} = \frac{1}{R} \begin{bmatrix} 3 & -1 & -1 & 0 & -1 \\ -1 & 3 & -1 & -1 & 0 \\ -1 & -1 & 4 & -1 & -1 \\ 0 & -1 & -1 & 3 & -1 \\ -1 & 0 & -1 & -1 & 4 \end{bmatrix}, \quad (42)$$

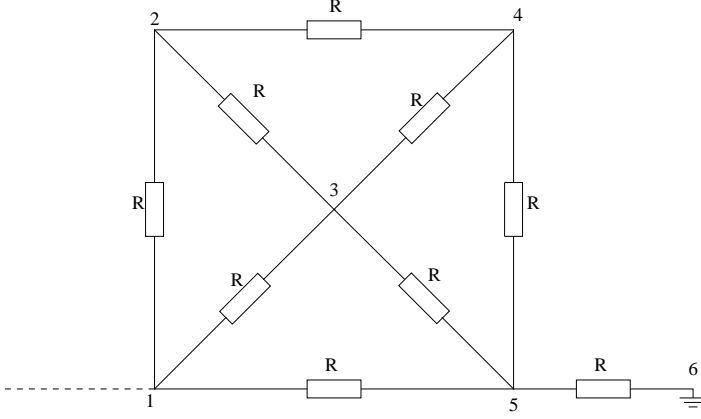


Figure 1: Electrical resistor circuit.

where we take all resistors to have the value $R = 100$.

To make this toy system non-linear, we add a global cubic non-linearity with an uncertain coefficient $(p_1 + 2)(\mathbf{u}^T \mathbf{u}) \mathbf{u}$. We also make the feed-in current $\mathbf{f} = (p_2 + 25)\mathbf{f}_0$ uncertain, so that we are eventually left to solve this system for \mathbf{u} (this is a concrete example of Eq. (1)):

$$\mathbf{A}(\mathbf{p}; \mathbf{u}) := (\mathbf{K}\mathbf{u} + (p_1 + 2)(\mathbf{u}^T \mathbf{u}) \mathbf{u}) = (p_2 + 25)\mathbf{f}_0 =: \mathbf{f}(\mathbf{p}), \quad (43)$$

$$\mathbf{f}_0 := [1, 0, 0, 0, 0]^T, \quad (44)$$

where the random parameters $\mathbf{p} = (p_1, p_2)$ are assumed uniformly and independently distributed in $[-1, 1]$, and therefore we have for the residuum (compare Eq. (3))

$$\mathbf{R}(\mathbf{p}; \mathbf{u}) = (p_2 + 25)\mathbf{f}_0 - (\mathbf{K}\mathbf{u} + (p_1 + 2)(\mathbf{u}^T \mathbf{u}) \mathbf{u}), \quad (45)$$

and for the preconditioner we take simply $\mathbf{P} = \mathbf{K} = \mathbf{D}_{\mathbf{u}}\mathbf{A}(\mathbf{p}; \mathbf{0})$.

The system can be solved in an iterative way as formulated in Eq. (2), with effectively

$$\begin{aligned} \mathbf{u}^{(k+1)} &= \mathbf{S}(\mathbf{p}; \mathbf{u}^{(k)}, \mathbf{R}(\mathbf{p}; \mathbf{u}^{(k)})) = \mathbf{u}^{(k)} + \mathbf{P}^{-1} \mathbf{R}(\mathbf{p}; \mathbf{u}^{(k)}) = \\ &\quad \mathbf{K}^{-1} \left((p_2 + 25)\mathbf{f}_0 - (p_1 + 2)((\mathbf{u}^{(k)})^T \mathbf{u}^{(k)}) \mathbf{u}^{(k)} \right) \end{aligned} \quad (46)$$

The simple iteration Eq. (46) — indeed a linearly convergent modified Newton method — converges quite well for the chosen parameters.

For the ansatz functions we take tensor products of Legendre polynomials, as they are orthogonal for the uniform measure, i.e. we take $\psi_\alpha(\mathbf{p}) = \tilde{L}_\alpha(\mathbf{p}) = L_\alpha(\mathbf{p})/\|L_\alpha\|$, the multi-variate normalised Legendre polynomial, and $L_\alpha(\mathbf{p}) = \prod_{i=1}^2 \ell_{\alpha_i}(p_i)$, where the ℓ_i are the normal univariate Legendre polynomials, $\|L_\alpha\| = 4(2\alpha_1 + 1)^{-1}(2\alpha_2 + 1)^{-1}$, and $\alpha \in (\mathbb{N}_0)^2$:

$$\mathbf{u}(\mathbf{p}) \approx \sum_{|\alpha|_1 \leq m} \mathbf{u}_\alpha \tilde{L}_\alpha(\mathbf{p}) =: \mathbf{u}_{\mathcal{I}}(\mathbf{p}), \quad \text{with} \quad (47)$$

$$\mathbf{u}_\alpha = [u_{\alpha,1}, \dots, u_{\alpha,5}]^T \in \mathcal{U} = \mathbb{R}^5, \quad \text{and}$$

$$\mathcal{I} = \{\alpha = (\alpha_1, \alpha_2) : |\alpha|_1 = \alpha_1 + \alpha_2 \leq m\} \subset (\mathbb{N}_0)^2, \quad m \in \mathbb{N};$$

hence for different $m \in \mathbb{N}$ we will have different approximation orders by polynomials of total degree m .

For the purpose of comparison we use two approaches to determine the coefficients \mathbf{u}_α in Eq. (47), these are the Galerkin approach according to Algorithm 4.2 with numerically integrated residuum according to Algorithm 4.1 for $\mathbf{u}_G(\mathbf{p})$, and collocation or more specifically discrete projection with numerical integration according to Algorithm 4.3 for $\mathbf{u}_C(\mathbf{p})$, both with the same integration rule. We choose here — as we are only in two dimensions — a tensor-product Gauss-Legendre quadrature. The quadrature order was always taken so that products of test- and ansatz-functions $\psi_\alpha \psi_\beta$ were integrated exactly for the chosen total polynomial degree m in Eq. (47).

First we computed a $N = 1000$ sample Monte Carlo solution on random points $\mathbf{p}_n \in \mathcal{P} = [-1, 1]^2, n = 1, \dots, N$ to high accuracy by setting the convergence criterion in Algorithm 2.1 to the machine tolerance. These results were taken as the reference solution for the following error estimation. We computed the root-mean-squared-error (RMSE) — effectively the L_2 norm in $\mathcal{Q} \otimes \mathcal{U} \cong L_2([-1, 1]^2; \mathbb{R}^5)$ — as

$$\epsilon_F = \left(\frac{1}{N} \sum_{n=1}^N \|\mathbf{u}(\mathbf{p}_n) - \mathbf{u}_F(\mathbf{p}_n)\|^2 \right)^{1/2}, \quad (48)$$

where the *functional approximation* method F is either G for the *Galerkin* method or C for the *collocation* method.

The two approaches were carried out to compute the coefficients \mathbf{u}_α in Eq. (47). The criteria of convergence for the iterative solvers were that the increment of \mathbf{u} or \mathbf{u}_α is smaller than ϵ_{tol} . Tabulated in Table 1 are the ϵ_{tol} values obtained in a sensitivity-range investigation such that further reduction of these values would not improve accuracy, depending on the total polynomial degree m . The errors ϵ_F of each approach were estimated as in

Order of poly- nomial	ϵ_{tol}	# of solver evals.		RMSE ϵ_F from Eq. (48)	
		Colloc.	Galerkin	$F = C$ Colloc.	$F = G$ Galerkin
m=2	10^{-6}	73	81	8.5×10^{-6}	8.2×10^{-6}
m=3	10^{-7}	151	160	6.4×10^{-7}	6.0×10^{-7}
m=4	10^{-8}	268	300	4.2×10^{-8}	4.0×10^{-8}
m=5	10^{-9}	430	468	3.1×10^{-9}	3.0×10^{-9}

Table 1: RMSE and number of solver evaluations of collocation and Galerkin approaches

Eq. (48) and are displayed in Table 1, together with the number of solver ($\mathcal{S}(\mathbf{p}, \mathbf{u})$) evaluations for total polynomial degrees $m = 2, 3, 4$ and 5. The coefficients computed by either Galerkin or collocation differed only in the eighth or ninth digit.

It is seen in the results that in terms of “the best possible accuracy” the Galerkin approach is slightly better than the collocation one, though the former needs slightly more evaluations of the solver. This comes because the same convergence tolerance is used for different equations in the two approaches. The results essentially confirm the theoretical analysis in Section 3; for the same accuracy both approaches need about the same number of solver calls, i.e. the simple block Jacobi iteration of the Galerkin system converges at essentially the same speed as the original iteration.

6 Conclusion

After reviewing the literature on numerical methods for parametric equations, with a special emphasis on the subclass of stochastic equations, we have introduced a general methodology to formulate numerical methods relying on functional or spectral approximations. We have shown that the Galerkin orthogonality conditions for the residuum and the iteration equation are equivalent under certain conditions, and that the simplest iterative scheme for the coupled Galerkin system, the block Jacobi method, converges essentially at the same speed as the original solver for a single parameter value.

In the main part for this “plain vanilla” Galerkin formulation, we have

shown how to approximate the preconditioned residuum in the Galerkin equation through numerical integration, and the effects of this on the iteration sequence. Then these explicit non-intrusive Galerkin algorithms have been compared on one simple, easy to understand, baby example. This showed that the theoretical analysis was validated with these computations, and that even in the simplest case of block Jacobi the Galerkin formulation is competitive with collocation. We finally recall once more the discussion in Section 4 on possibilities to accelerate the coupled Galerkin solution, something that is not possible for the decoupled collocation approach.

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